Schedule

9:30-10:00 Registration.

10:00-10:05 **Prof Dominic Vella**, University of Oxford, Opening Remarks.

10:05-10:50 **Prof Julia Yeomans**, University of Oxford, *Active nematics: topology in biology.*

10:50-11:10 **James Kwiecinski**, University of Oxford, *Self-assembly in mechanical systems.*

11:10-11:30 **Alice Schwarze**, University of Oxford, *Redundancy, degeneracy, and robustness in protein-interaction networks.*

11:30-12:00 Coffee Break

12:00-12:20 **Sean Lim**, University of Oxford, *An introduction to Bayesian inverse problems.*

12:20-12:40 **Marco Agnese**, Imperial College London, *Fitted finite element discretization of two-phase Navier-Stokes flow.*

12:40-13:00 **Jamie Taylor**, University of Oxford, *Convex duality methods for a non-convex minimisation problem.*

13:00-14:00 Lunch Break

14:00-14:30 Poster Session

14:30-14:50 **Anton Mühlemann**, University of Oxford, *On optimal lattice transformations.*

14:50-15:10 **Stuart Thomson**, University of Oxford, *Violent elastic-plastic wave interactions.*

15:10-15:30 **Matthew Saxton**, University of Oxford, $\sqrt{t}$*, or not* $\sqrt{t}$*, that is the question.*

15:30-15:50 **Doireann O'Kiely**, University of Oxford, *Stretching and buckling of thin viscous sheets.*

15:50-16:20 Coffee break

16:20-16:40 **Paul Taylor**, University of Oxford, *Random walks and volume-exclusion: reconciling models of diffusive transport across scales.*

16:40-17:25 **Prof Mike Giles**, University of Oxford, *Multilevel Monte Carlo methods.*

17:25-17:40 Closing Remarks/Awards

17:40-19:00 Pizza and Drinks in the Common Room

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Talks

1. **James Kwiecinski**, University of Oxford
   Self-Assembly in mechanical systems

   The presentation will focus on the shaping of biological membranes, in particular lipid bilayers, by means of curvature-inducing proteins. The lipid bilayer is an important building block at the cellular level, coating certain parts of the cell, such as the nucleus, and forming independent biological objects, such as vesicles which are responsible for the transport of waste and nutrients in the cell. The shape of these resultant entities is fundamental to their function, so the self-assembly process, and the understanding thereof, is of utmost biological importance.

   Mathematically, this self-assembling system forms a fascinating interaction process because such proteins act as curvature sensors; that is, the shape of the membrane determines where the proteins attach onto and cause the membrane to curve. This, in turn, affects further protein attachment.

   By deriving a model from mechanical principles, in particular, from continuum and statistical mechanics, we can ask fundamental questions about the system, such as the dependence of the self-assembly process on experimental parameters and the existence and stability of possible membrane shapes. We use weakly nonlinear analysis to show that pattern formation in protein aggregation is possible for certain chemical triggers and consider the role of competing protein processes in the final membrane configuration.

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2. **Alice Schwarze**, University of Oxford
   Redundancy, degeneracy, and robustness in protein-interaction networks

   Researchers in *network pharmacology* model complex biological systems as networks and use tools from network analysis to gain insights in biological problems. This approach can facilitate multi-target drug discovery. For example, one can associate biological systems with protein-interaction networks (PINs) and chemical compounds affecting these systems with network perturbations. By analysing the structural changes induced by such a perturbation on a PIN, it is possible to elucidate the systemic impact of a chemical compound on a biological system.

   It is unclear how biological function relates to structural properties of the corresponding PINs. A better understanding of this relationship is needed to define suitable

impact measures for perturbations that network pharmacologists use to model the impact of a drug on a biological system.

In collaboration with e-therapeutics, we aim to find computational methods for identifying structural properties that may be linked to the integrity of biological functions in a cell. For this purpose, we identify links between biological and structural robustness of PINs. To that end, we combine insights from evolutionary biology on the robustness of complex biological systems with findings on the percolation properties of PINs and random graph models thereof.

The relationship between structure and function of biological networks has been of considerable interest to researchers in neuroscience. For PINs, we adapt a method that Tononi et al. [1] proposed for linking the structure of cortical networks to biological characteristics: We use information-theoretic measures for quantifying biological redundancy and degeneracy — two concepts that evolutionary biologists consider to be closely linked to robustness of biological systems — and link these quantities to small-scale structures (graphlets) in PINs.

[1] G. Tononi, O. Sporns, and G. M. Edelman, *Measures of degeneracy and redundancy in biological networks*, Proceedings of the National Academy of Sciences USA, vol. 96, no. 6, pp. 3257–3262, 1999.

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3. **Sean Lim**, University of Oxford
An introduction to Bayesian inverse problems

In many applications, inverse problems are solved. We adopt a statistical approach, working within the Bayesian framework to solve inverse problems. The solution of an inverse problem is given by a posterior measure. One is then left with the task of interpreting the posterior measure. We explore some methods to explore the posterior density and give some examples.

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4. **Marco Agnese**, Imperial College London
Fitted finite element discretization of two-phase Navier-Stokes flow

We propose a novel fitted finite element method for two-phase Navier-Stokes flow problems that uses piecewise linear finite elements to approximate the moving interface. The meshes describing the discrete interface in general do not deteriorate in time, which means that in numerical simulations a smoothing or a remeshing of the

interface mesh is not necessary. We present several numerical experiments for our numerical method, which demonstrate the accuracy and robustness of the proposed algorithm.

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5. **Jamie Taylor**, University of Oxford
Convex duality methods for a non-convex minimisation problem

The Onsager model is a classical description of phase transitions in liquid crystalline systems that is still of great significance in contemporary research. The model is phrased as a minimisation problem, which to have interesting so- lutions must be non-convex. In this work, a general method for applying convex duality methods to such models will be presented, based on the observation that the objective function is convex on a set of finite codimension. This allows the infinite-dimensional minimisation problem to be reduced to a smooth, finite- dimensional min/max problem which is fully equivalent to the original problem from the perspective of equilibrium configurations. This formulation rephrases tougher questions from functional analysis in terms of multivariable calculus, allowing one to use simpler techniques to obtain rigorous results. Furthermore the finite dimensional problem is stable, in the sense that approximate solutions can be used to obtain approximate solutions to the original model, leading to effective methods for solving the method numerically.

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6. **Anton Mühlemann**, University of Oxford
On optimal lattice transformations

A group of objects, arranged in a regular and periodic configuration, is forced to rearrange itself homogeneously into a different periodic structure. Out of the arbitrarily many ways of doing so, which is the one requiring the least movement?

This question is particularly relevant in displacive phase transitions in crystalline solids. There, the objects could be atoms which are forced into a new crystalline structure due to changes in temperature.

In this talk I will introduce a suitable framework and use it to prove a conjecture by E.C. Bain from 1924 concerning phase transformations in steels. [1] Koumatos,

K. and Mühlemann, A., Optimality of general lattice transformations with applications to the Bain strain in steel, Proceedings of the Royal Society A: Mathematical, Physical & Engineering Sciences, London, 2016

7. **Stuart Thomson**, University of Oxford
Violent elastic-plastic wave interactions

In isentropic compression experiments, millimetre thick metal samples are subjected to pressures on the order of $10 - 10^2$ GPa, while the yield strength of the material can be as low as 10^{-1} GPa. In such regimes the metal can be treated as a barotropic compressible fluid in which the strength, measured by the ratio of the yield stress to the applied stress, is negligible to lowest order. We present a new model of elastoplasticity which incorporates the effects of strength as a small perturbation to the leading order model based on barotropic flow. We then consider the elastic/plastic waves that propagate through the metal sample and the consequences of their interactions on obtaining equation of state information for the highly plasticised metal.

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8. **Matthew Saxton**, University of Oxford
$\sqrt{t}$, or not $\sqrt{t}$, that is the question

We consider the motion of a thin liquid drop on a smooth substrate as the drop evaporates into an inert gas. Many experiments suggest that, at times close to the drop's extinction, the drop radius scales as the square root of the time remaining until extinction. However, other experiments observe slightly different scaling laws. We use the method of matched asymptotic expansions to investigate whether this different behaviour is systematic or an artefact of experiment.

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9. **Doireann O'Kiely**, University of Oxford
Stretching and buckling of thin viscous sheets

Thin glass sheets are used in smartphone, battery and semiconductor technology, and may be manufactured by producing a relatively thick glass slab and subsequently redrawing it to a required thickness. The resulting sheets commonly possess undesired centreline ripples and thick edges. We present a mathematical model in which a viscous sheet undergoes redraw in the direction of gravity, and show that, in a sufficiently strong gravitational field, buckling is driven by compression in a region near the bottom of the sheet. We use asymptotic analysis in the thin-sheet, low Reynolds number limit to determine the centreline profile and growth rate of such a viscous sheet.

10. **Paul Taylor**, University of Oxford
Random walks and volume-exclusion: reconciling models of diffusive transport across scales

Diffusion is integral to many biological processes, and stochastic lattice-based position-jump models are a popular choice for interrogating diffusive systems. A balance must sometimes be found between precise, but computationally intensive, fine-grained models, and approximate, coarse-grained models which can be simulated in a fraction of the time.

In this talk, I outline both coarse- and fine-grained lattice models of diffusion which incorporate volume exclusion, and how the connection between the two can be demonstrated. I also illustrate hybrid models combining coarse- and fine-grained regions. These hybrid models take less time to simulate than exclusively fine-grained models, but provide increased accuracy compared to coarse-grained models in some scenarios.

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Posters

Casper Beentjes, University of Oxford
Position determination by a single cell using chemical sensing

Cells like spermatozoa or neural axons have to be able to find targets over a large range of length scales. The process of chemoreception could serve as a mean for cells to direct their movement through a medium. Many studies since the seminal paper by Berg and Purcell have looked into mathematical models and limitations of chemotaxis. Literature, however, overlooks the actual influence of the position of the source relative to the cell and the question whether directional information can be extracted from diffusing molecules. In this work, joint with David Holcman and Radek Erban, we address the question how mathematically a long-range guidance of cells using chemoreception can be established. In particular we look at the influence of the geometry of the cell, receptor and source on the sensitivity of the receptors and the question, can a cell determine the precise location of a target source? As the receptors are small in size relative to the cell membrane this allows for the use of a perturbation approach in the form of the small hole and narrow escape theory. A new computational approach is set out which focuses computational resources on the part of the domain close to the cells by making use of the first-passage formalism of diffusing particles inspired by the Green's Function Reaction Dynamics method.

Niall Bootland, University of Oxford
Preconditioners for incompressible two-phase flow

Two-phase flows arise in many coastal and hydraulic engineering applications such as the study of coastal waves, dam breaking scenarios, and the designing of channels and coastal structures. However, modelling two-phase incompressible flow with level set or volume-of-fluid formulations results in a variable coefficient Navier-Stokes system that is challenging to solve computationally. In this poster we consider block preconditioners for such two-phase Navier-Stokes systems by looking to adapt efficient preconditioners for one-phase Navier-Stokes flows. In particular we consider systems arising from the application of finite element methodology and preconditioners which are based on approximate block factorisations. A crucial ingredient is a good approximation of the Schur complement arising in the factorisation which can be computed efficiently.

Ferran Brosa Planella, University of Oxford
Microstructure modelling in solidification of silicon

Elkem are interested in improving their silicon casting processes to achieve a final product that better fits their customers needs. The focus of this research project is to develop a mathematical model that will explain some of the behaviour of the microstructure that is created during the solidification process in silicon. This model should lead to a better understanding of the solidification process and to an improvement of the casting methods and the quality of the product. Because the silicon has significant concentrations of numerous impurities in it the model takes into account of possible intermetallic phases that can be created and the constitutional supercooling that can occur during the solidification of silicon. The initial studies presented here employ asymptotic techniques to obtain approximate solutions which give us a better understanding of the casting process of silicon.

Roxana Feier, University of Oxford
Community detection in product–purchase networks

A successful programme of personalised discounts and recommendations relies on identifying products that customers want, based both on items bought in the past and on relevant products that the customers have not yet purchased. Using basket-level grocery shopping data, we aim to identify groups of shoppers with similar preferences, along with the corresponding products that they purchase, to design better recommendation systems.

We model the customers and products as nodes in a weighted, bipartite network and we use a class of clustering methods from network theory known as community detection to find structure in the data. Roughly speaking, communities are sets of nodes (which here include both customers and products) that are more densely connected with each other than with other nodes in the network. We used a suite of standard similarity measures to compare different partitions of the same network into communities and we found, for instance, that different weightings along the network edges produce weakly related community structure. Finally, using hypothesis testing, we identified a group of customers in a small convenience store that are particularly sensitive to promotions.

Rachel Philip, University of Oxford
Modelling oil droplet formation in turbulent oil plumes

In deepsea oil extraction an accidental blow-out (an uncontrollable release of oil into the sea) can cause significant environmental damage. In such an oil spill, a broken pipe at the seabed releases a highly turbulent jet of oil into the water. The oil drops produced in this plume rise to the surface of the sea and form a oil slick, which can be difficult to clean up. It is advantageous to use the vigorous turbulent mixing of the plume to break up oil drops and produce smaller drops. These smaller oil droplets can then be eaten by naturally occurring microbes in the sea, and thereby are removed from the water column before reaching the surface.

Modelling oil droplet breakup is a challenge since it involves examining and unifying disparate macroscopic and microscopic scales. The macroscopic plume is made up of large and small turbulent eddies. On the smaller scale, we consider microscopic droplets which can be deformed and broken up by these eddies of different sizes. We separately model the plume, using turbulence models, and the droplet scale, using statistical and dimensional models as well as fluid dynamical models of drop eddy interactions. These scales are connected by breakup parameters, which are used in the microscopic droplet breakup models and depend on macroscopic flow properties. By combining these macroscopic and microscopic models, we produce droplet population distributions. In this poster, we use these models to provide insights into the factors affecting droplet breakup.

Ben Sloman, University of Oxford
Mathematical evaluation of optimal design of silicon furnaces

Elkem Silicon Materials are one of several global companies who produce silicon by feeding quartz rock and carbon into huge furnaces, which are heated by electrodes. Through this research we seek to understand furnace behaviour better, in order to improve the efficiency of production. Several chemical reactions occur, as well as interactions between solid, liquid and gaseous phases. The high temperatures found (around 2000 kelvin) are influenced by the chemical reactions and electrical heating. Mathematical modelling is crucial to understand the interdependence between these important physical and chemical effects. Models are developed using continuum approaches, and numerical methods are utilised to determine how the chemical concentrations and temperature vary in time and space in the furnace.